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Prediction of Heavy Element Fission Barrier Features for Multiple Chance Nuetron Cross-Section Calculations

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ABSTRACT

A state of the art calculation of even, odd, and even-odd heavy neutron-rich element fission barriers and neutron binding energies is described. The range $76 \leq Z \leq 100$, $118 \leq N \leq 184$ is selected for application to ICF burnup. Some techniques for exploring multi-dimensional parameter spaces on the computer are discussed. Contour maps of fission barriers and neutron binding energies are shown.

Heavy element production calculations via neutron capture processes in laser fusion pellets or underground thermonuclear explosions require extensive knowledge of the nuclear properties of a broad range of neutron-rich heavy elements. Such knowledge is also needed for the burnup of radioactive wastes in ICF pellets by a neutron spectrum centered near 14 MeV and extending to 20 MeV, a process which has recently been considered[1] for nuclear waste management.

For these highly neutron-rich nuclei, the neutron emission threshold decreases to a few MeV, so that up to fourth or higher chance fission competition may be required, in the above bombarding energy range. These calculations use statistical theory methods as implemented in the TNG code of Fu.[2] One of the more important inputs for these codes is a set of consistent neutron binding energies and multiple barrier heights for the relevant elements of a chain.

We have calculated fission barriers and ground state masses for some 2000 elements with $76 \leq Z \leq 100$ and $118 \leq N \leq 184$ (for even, odd, and odd-even nuclei) using the well-known macroscopic-microscopic model.

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The single-particle energies and pairing correlations come from the modified oscillator potential while the droplet model supplies the macroscopic energy. The calculation closely follows the corresponding one discussed in References 3 and 4, where additional references can be found. The present effort includes a zero-point energy of about 0.5 MeV, ε_2, ε_3, ε_4, and ε_5 degrees of freedom and γ degrees of freedom when appropriate and to this extent represents the state of the art for this type of fission barrier modeling. This technique was found[3,4] to predict fission barriers in good agreement with the available data. Here, however, we must keep in mind that we are extending the calculation to a wide range of nuclei not available to ordinary experiment. Some caution will therefore be in order when interpreting the results of actinide burnup predictions.

One major uncertainty in this calculation of fission barriers and particle emission thresholds for neutron-rich heavy elements is the value of the surface asymmetry term in the expression for the macroscopic energy; that is, how rapidly the surface energy is reduced as a function of increasing neutron number. For the calculations reported here, we chose the droplet model for the macroscopic energy. A recent evaluation employing a "new macroscopic" model[5] finds that the surface energy is reduced much less rapidly as a function of increasing neutron number than predicted by the droplet model. This effect will mean that the fission thresholds may decrease less rapidly as a function of neutron number than our calculations suggest. A new calculation of fission barriers employing this macroscopic model is underway.

As in References 3,4, we first determine the saddle points and minima by considering symmetric elongation and necking coordinates only (ε_2 & ε_4). For $\varepsilon_2 \leq 0.65$ we next determine the decrease in the calculated fission barrier heights arising from the mass-asymmetric (ε_3 & ε_5) deformations. In the lower region $0 \leq \varepsilon \leq 0.60$ the decrease of the (ε_2 , ε_4) fission barriers comes mostly from the γ degree of freedom rather than the (ε_3, ε_5) ones; only the γ deformations are therefore considered there. Still, we see that for each nucleus three two-dimensional potential energy surfaces are calculated. Since thousands of nuclei have been considered, it was necessary to develop computer codes using novel techniques for finding saddle points and minima and for merging the results from the three surfaces into a single one-dimensional fission barrier curve. These codes are now briefly described.

The minima and saddle points are to be determined from a 10 x 10 table containing energies vs. ε_2 and ε_4. A fine grid of about 50 x 120 points is generated by interpolation of the starting table. At each point on the grid one looks at the eight nearest neighbors to determine the sign of the change in the function from the chosen point and its neighbors. Some typical results are shown in Figure 1.

- - -	+ + +	+ + +	+ + +	+ + +
- 0 -	+ 0 +	+ 0 -	+ 0 -	+ 0 -
- - -	+ + +	+ - +	- + +	+ - -
(1a)	(1b)	(1c)	(1d)	(1e)

Figure 1

The configuration (1a) shows that our current point is a maximum point, while (1b) indicates a minimum. Next (1c) and (1d) represent saddle points while (1e) is a point on a slope and is therefore discarded. By identifying the patterns in this manner, all minima and saddle points were found. The required path consists of those points ordered by increasing value of ε_2, for the $(\varepsilon_2, \varepsilon_4)$ case, and so on for the other surfaces.

To merge the results from the three surfaces we start with the fission path in the symmetric $(\varepsilon_2, \varepsilon_4)$ surface. Then for $\varepsilon_2 \lesssim 0.60$ we next replace the symmetric peaks and minima by the corresponding saddles and minima in the $(\gamma, (\varepsilon_2, \varepsilon_4(\varepsilon_2)))$ plane, provided they have lower energy. For $\varepsilon_2 \lesssim 0.65$ a similar procedure for the $[(\varepsilon_3, \varepsilon_5 (\varepsilon_2, \varepsilon_4)),(\varepsilon_2, \varepsilon_4 (\varepsilon_2))]$ plane. Here the independent variables of the plane are ε_3 and ε_2; ε_4 depends on ε_2 as in the first minimization and ε_5 is taken to be the one which minimizes the energy for the given ε_2 ε_4 pairs. When one adds details pertaining to file and table generation the merging programs represents some 1000 FORTRAN statements. Since our original aim was to find the minimal path in the five-dimensional ε_2, γ, ε_3, ε_4, ε_5 space, a task which could easily get out of hand, the present solution is relatively fast and simple to apply.

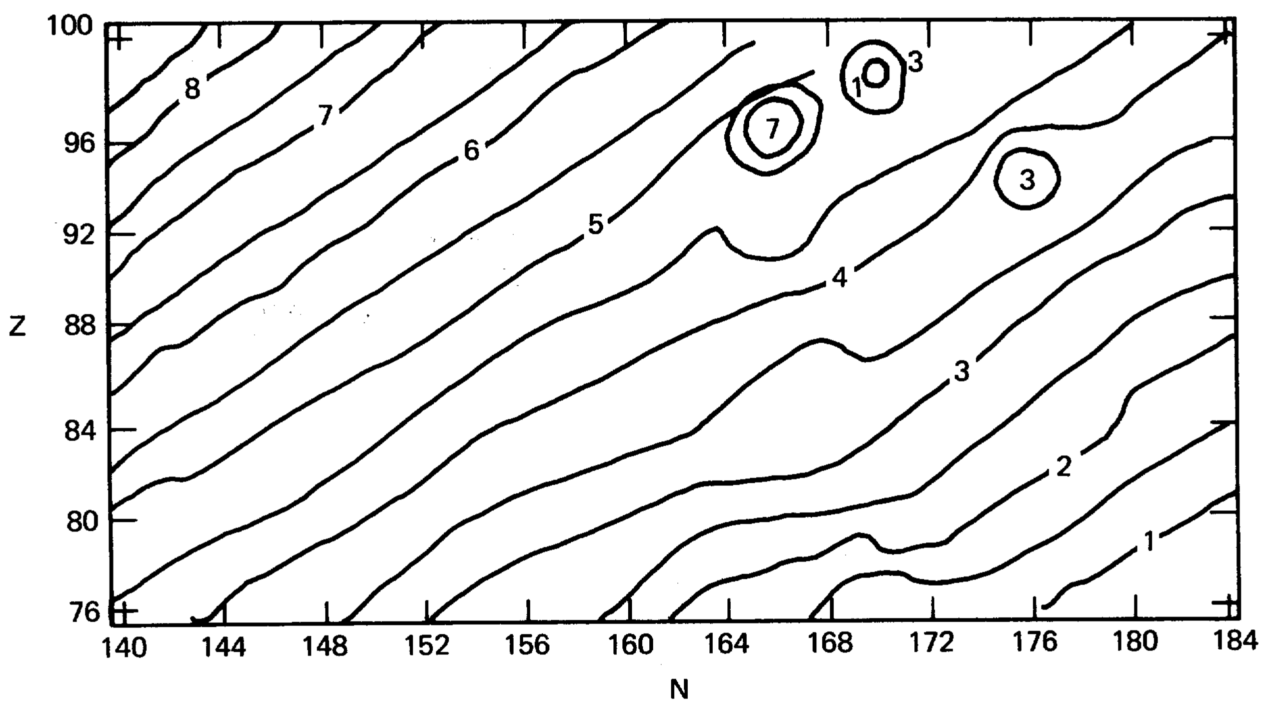
The results to be published[6] include two detailed tables. One table gives the fission barrier height, particle separation energies, and the beta decay energies for each nucleus. The second table gives the structure of the nuclear potential energy surface for each nucleus, including the energy and shape for each maximum and minimum. These results are summarized in Figures 2 and 3.

Figure 2 is a contour plot of the neutron separation energy for even nuclei in the region $76 \leq Z \leq 100$ and $140 \leq N \leq 184$. The number on the contour line is the separation energy in MeV. One observes the standard decrease in neutron binding energy as a function of increasing neutron number. An unusual features of this plot is the presence of local maxima and minima near Z = 96 and N = 166, 170 and 176. These features are due to large ground state shape changes upon emission of a single neutron.

Figure 3 is a contour plot of the fission barrier height (including 0.5 MeV zero-point energy) for even nuclei in the region $76 \leq Z \leq 100$ and $140 \leq N \leq 184$. Again the distance between contours is 0.5 MeV and the integer contours are labelled in MeV. One observes the well-known "Bay of Pigs" features at $A \simeq 92$ and $160 \leq N \leq 176$. This arises as a result of the changing Nilsson energy levels configurations in this region, and can have a profound effect on the production of heavy neutron-rich elements in a thermonuclear environment, as well as on burnup in ICF, thus underscoring the importance of understanding the detailed structure of these heavy elements.

Additional details and the full table of results will be published[6] in <u>Atomic and Nuclear Data Tables</u>. Multiple chance fission calculations using these tables are currently in progress.[7]

Figure 2



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148
152
156
160
164
168
172
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184
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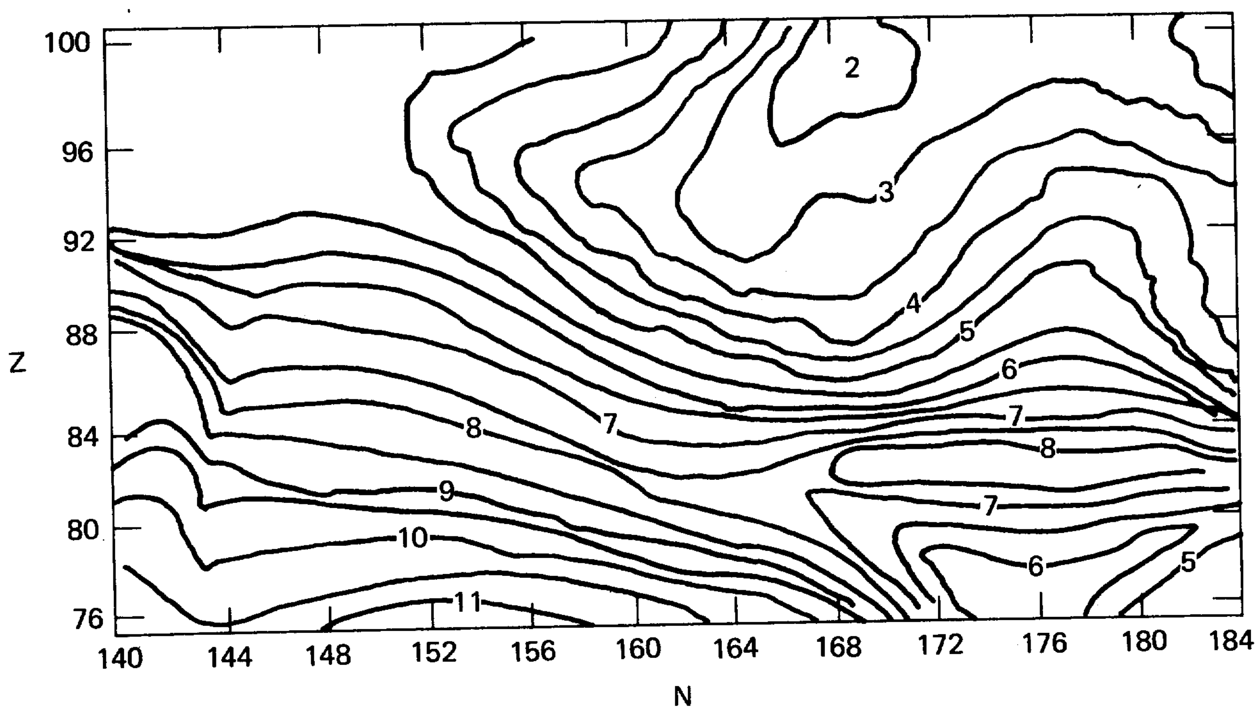
Figure 3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